Project H-15: Complex hydride compounds with enhanced hydrogen storage capacity

D.L. Anton
United Technologies Research Center, E. Hartford, CT, USA
E-mail: ANTONDL@UTRC.UTC.COM

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Background

The state-of-the-art material for chemical hydrogen storage is sodium aluminum tetrahydride ($NaAlH_4$), which, when catalyzed with transition metal cations, has been shown to approach the required hydrogen desorption and absorption rates required for operating polymer electrolyte membrane fuel cell powered automobiles. This complex hydride has a total practical hydrogen storage capacity of 5.5 wt %. In determining the specifications for a chemical hydrogen storage system, the media hydrogen mass must be taken as a fraction of the total hydrogen storage system weight including both the hydrogen storage medium and the system components. In order to meet the 6 wt% system goal, and assuming a 80-85% gravimetric engineering efficiency (mass of media/[mass of media+system]), a new chemical hydride material with a hydrogen weight fraction of 7-7.5wt % will be needed. The goal of the proposed project is to develop a new complex hydride compound capable of reversibly storing a hydrogen capacity of $\geq$7.5 wt % and of capacity regeneration for 500 cycles with 100 % efficiency.

Project Plan

The objective of this new (2004) project is to discover new reversible high hydrogen content complex hydride compounds, $Na_yM^{+i}{}_x(AlH_4)_{y+ix,}$ in the quaternary phase space between sodium hydride (NaH), alane (AlH_3), transition metal or rare earth (M) hydrides (MH_z, where z = 1-3) and molecular hydrogen (H_2). This project will encompass all of the technology development stages for identifying, developing and commercializing complex hydride compound hydrogen storage media to meet the required DOE performance targets. United Technologies Research Center will lead an international team including Savannah River Technology Center (SRTC), Albemarle Corp. and IFE (Norway) with an accomplished portfolio of capabilities in solid-state modeling, inorganic syntheses, materials structural characterization, hydrogen storage performance evaluation, chemical cost reduction, manufacturing scale-up and fuel cell system development and business analyses. The team will accelerate the discovery of new complex hydride compounds and guide experimentation with first principles modeling. Simultaneously, the team will apply multiple synthetic methodologies to isolate new hydrides, and couple thermodynamic predictions and structural characterizations to verify structures of newly identified phases. The team will conduct three levels of performance evaluations to select compositions for further development, optimize dehydrogenation and hydrogenation catalysis with spectroscopic mechanistic studies and first-principles screening simulations, develop manufacturing processes to reduce cost and scale-up production, and develop business analyses for the commercialization of hydrogen storage systems integrated with fuel cell power plants.